



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:24 PM UTC

PDB ID : 2PGG / pdb_00002pgg
Title : Crystal Structure of a Birnavirus (IBDV) RNA-dependent RNA Polymerase VP1
Authors : Pan, J.; Vakharia, V.N.; Tao, Y.J.
Deposited on : 2007-04-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

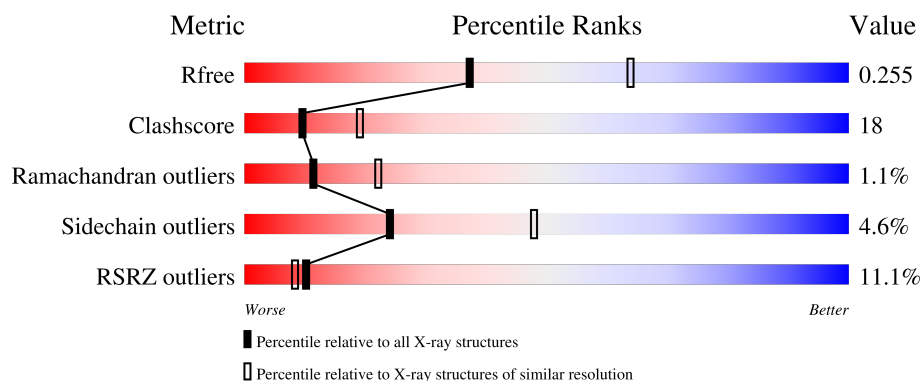
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	774	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6447 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6020	3848	1014	1136	22			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	427	Total	O	0	0
			427	427		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.10Å 122.10Å 359.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.97 – 2.50 39.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.97-2.50) 96.4 (39.97-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.254 0.217 , 0.255	Depositor DCC
R_{free} test set	3267 reflections (6.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6447	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/6164	0.93	21/8377 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	LEU	N-CA-C	-7.31	99.46	110.28
1	A	185	GLY	N-CA-C	7.11	118.21	111.67
1	A	761	LYS	CA-C-N	6.55	126.49	119.28
1	A	761	LYS	C-N-CA	6.55	126.49	119.28
1	A	63	GLN	N-CA-C	-6.53	99.90	109.50
1	A	352	THR	N-CA-C	6.50	119.33	111.40
1	A	124	TYR	CA-C-N	6.50	124.40	119.66
1	A	124	TYR	C-N-CA	6.50	124.40	119.66
1	A	428	HIS	N-CA-C	-6.29	104.34	111.07
1	A	560	GLU	N-CA-C	-6.05	106.51	114.31
1	A	715	ALA	N-CA-C	-5.83	104.84	111.14
1	A	634	TYR	CA-C-N	5.51	126.73	119.84
1	A	634	TYR	C-N-CA	5.51	126.73	119.84
1	A	260	LEU	N-CA-C	5.49	121.95	109.81
1	A	537	ILE	N-CA-C	5.38	116.16	110.72
1	A	547	LEU	N-CA-C	5.35	119.50	112.92
1	A	240	ASP	N-CA-C	-5.34	107.13	113.97
1	A	785	ILE	N-CA-C	-5.25	107.86	112.90
1	A	573	TRP	N-CA-C	5.21	118.23	109.95
1	A	566	VAL	N-CA-C	-5.08	100.33	107.75
1	A	205	LEU	N-CA-C	-5.04	105.50	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6020	0	6033	214	1
2	A	427	0	0	18	0
All	All	6447	0	6033	214	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:THR:HG23	1:A:724:ARG:H	1.11	1.11
1:A:429:MET:HE2	1:A:492:ASN:HD21	1.21	1.02
1:A:412:TRP:HB2	1:A:537:ILE:HD12	1.43	0.99
1:A:429:MET:HE2	1:A:492:ASN:ND2	1.81	0.96
1:A:612:VAL:HG13	1:A:613:GLY:H	1.32	0.92
1:A:191:ASP:CG	1:A:427:GLN:HG3	1.98	0.88
1:A:209:THR:HG21	1:A:498:THR:OG1	1.75	0.84
1:A:486:ASN:O	1:A:489:THR:HG22	1.77	0.84
1:A:356:MET:HE3	1:A:491:ILE:HD11	1.60	0.83
1:A:78:ILE:HG22	1:A:79:LEU:HD22	1.63	0.81
1:A:329:THR:HG23	1:A:333:LYS:HB3	1.62	0.81
1:A:425:THR:HG22	1:A:428:HIS:H	1.47	0.79
1:A:722:THR:HG23	1:A:724:ARG:N	1.95	0.78
1:A:425:THR:HG23	1:A:427:GLN:HE21	1.50	0.76
1:A:425:THR:CG2	1:A:427:GLN:HG2	2.15	0.75
1:A:412:TRP:CB	1:A:537:ILE:HD12	2.17	0.75
1:A:425:THR:HB	1:A:428:HIS:HD2	1.50	0.75
1:A:356:MET:HE1	1:A:436:ILE:CD1	2.17	0.75
1:A:323:GLU:HG3	2:A:1318:HOH:O	1.86	0.74
1:A:429:MET:HE1	1:A:465:VAL:CG2	2.20	0.72
1:A:616:GLN:HB2	1:A:652:LEU:HD21	1.71	0.72
1:A:110:TYR:CE2	1:A:112:PRO:HG3	2.25	0.71
1:A:516:GLU:HG3	2:A:1104:HOH:O	1.91	0.71
1:A:429:MET:HE1	1:A:465:VAL:HG23	1.73	0.71
1:A:86:ARG:HA	1:A:91:ALA:HB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:HE2	1:A:477:ILE:CG2	2.06	0.67
1:A:425:THR:HB	1:A:428:HIS:CD2	2.28	0.67
1:A:586:PRO:HD2	1:A:694:ASN:HD21	1.59	0.67
1:A:227:ARG:HB2	1:A:232:MET:HE2	1.76	0.67
1:A:362:ASN:C	1:A:362:ASN:HD22	2.02	0.67
1:A:719:ALA:O	1:A:722:THR:HG22	1.95	0.66
1:A:238:ASP:C	1:A:240:ASP:H	2.03	0.66
1:A:260:LEU:CD2	1:A:315:CYS:HB3	2.25	0.66
1:A:527:ASN:HD22	1:A:527:ASN:N	1.95	0.65
1:A:511:ARG:HH11	1:A:511:ARG:HB3	1.60	0.65
1:A:356:MET:HE1	1:A:436:ILE:HD11	1.79	0.65
1:A:146:GLU:HG3	2:A:1344:HOH:O	1.96	0.65
1:A:266:THR:OG1	1:A:269:GLU:HG3	1.97	0.65
1:A:616:GLN:HG3	1:A:651:HIS:HD2	1.62	0.65
1:A:586:PRO:HD2	1:A:694:ASN:ND2	2.12	0.64
1:A:321:LYS:HE3	1:A:323:GLU:OE1	1.98	0.64
1:A:324:ARG:NH1	1:A:599:TYR:O	2.29	0.64
1:A:208:ILE:HD11	1:A:709:ASN:HB3	1.79	0.64
1:A:291:GLN:HE22	1:A:302:LYS:HD2	1.61	0.64
1:A:206:LEU:HD11	1:A:495:LEU:HD22	1.80	0.64
1:A:566:VAL:HG12	1:A:568:LEU:HD13	1.80	0.63
1:A:485:GLY:H	1:A:489:THR:HG21	1.64	0.62
1:A:187:ASN:HD22	1:A:527:ASN:ND2	1.97	0.62
1:A:425:THR:HG21	1:A:427:GLN:HG2	1.81	0.62
1:A:356:MET:HE1	1:A:436:ILE:HD12	1.80	0.62
1:A:185:GLY:HA2	2:A:1166:HOH:O	1.99	0.62
1:A:252:ILE:HD11	1:A:267:LYS:HD3	1.82	0.62
1:A:616:GLN:HG3	1:A:651:HIS:CD2	2.34	0.61
1:A:116:PRO:HB2	1:A:121:PRO:HA	1.83	0.61
1:A:181:GLU:O	1:A:184:THR:O	2.18	0.61
1:A:704:VAL:HG12	1:A:705:ASN:N	2.14	0.61
1:A:745:GLN:HG2	2:A:1256:HOH:O	2.01	0.61
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.82	0.60
1:A:714:LYS:HB2	2:A:1418:HOH:O	2.01	0.60
1:A:462:PRO:HB2	1:A:794:LEU:HD21	1.82	0.60
1:A:778:ASP:O	1:A:782:LYS:HG2	2.00	0.60
1:A:191:ASP:OD1	1:A:427:GLN:HG3	2.02	0.60
1:A:291:GLN:NE2	1:A:302:LYS:HD2	2.17	0.60
1:A:771:GLU:OE1	1:A:772:ARG:HD2	2.02	0.60
1:A:425:THR:HG23	1:A:427:GLN:HG2	1.85	0.59
1:A:65:ARG:HD3	1:A:476:GLN:OE1	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HB	1:A:244:GLU:HB3	1.85	0.58
1:A:667:SER:O	1:A:673:GLY:HA3	2.03	0.58
1:A:198:THR:H	1:A:201:SER:HB3	1.68	0.58
1:A:722:THR:HA	2:A:1475:HOH:O	2.03	0.58
1:A:382:LEU:HD22	1:A:586:PRO:HA	1.85	0.58
1:A:41:GLU:O	1:A:43:PRO:HD3	2.03	0.58
1:A:226:THR:HA	1:A:450:ASN:ND2	2.19	0.57
1:A:145:ASN:ND2	1:A:147:GLY:H	2.02	0.57
1:A:362:ASN:H	1:A:365:ASN:HD21	1.50	0.57
1:A:35:LYS:HG2	2:A:1121:HOH:O	2.05	0.57
1:A:531:GLU:OE1	1:A:532:ARG:HB2	2.05	0.57
1:A:482:GLN:OE1	1:A:489:THR:HA	2.05	0.56
1:A:447:PRO:O	1:A:448:MET:HE2	2.05	0.56
1:A:291:GLN:OE1	1:A:299:ASN:HB3	2.06	0.56
1:A:425:THR:HG22	1:A:428:HIS:N	2.20	0.56
1:A:704:VAL:HG12	1:A:705:ASN:H	1.70	0.56
1:A:145:ASN:HD22	1:A:145:ASN:C	2.13	0.56
1:A:362:ASN:ND2	1:A:364:LEU:H	2.04	0.54
1:A:295:THR:HG21	2:A:1491:HOH:O	2.07	0.54
1:A:85:MET:SD	1:A:233:LEU:HD13	2.47	0.54
1:A:324:ARG:NH2	1:A:671:GLU:OE1	2.41	0.54
1:A:486:ASN:O	1:A:489:THR:CG2	2.53	0.53
1:A:427:GLN:H	1:A:427:GLN:CD	2.16	0.53
1:A:324:ARG:HH22	1:A:671:GLU:CD	2.16	0.53
1:A:59:TYR:CE2	1:A:477:ILE:CG2	2.91	0.53
1:A:427:GLN:H	1:A:427:GLN:NE2	2.06	0.53
1:A:60:LYS:HE3	2:A:1270:HOH:O	2.09	0.52
1:A:511:ARG:HH11	1:A:511:ARG:CB	2.20	0.52
1:A:59:TYR:HE2	1:A:477:ILE:HG23	1.74	0.52
1:A:260:LEU:HD22	1:A:315:CYS:HB3	1.89	0.52
1:A:612:VAL:HG13	1:A:613:GLY:N	2.12	0.52
1:A:180:LYS:NZ	2:A:1152:HOH:O	2.42	0.52
1:A:382:LEU:HD22	1:A:586:PRO:CA	2.40	0.52
1:A:504:TRP:CD1	1:A:510:PRO:HD2	2.45	0.51
1:A:238:ASP:C	1:A:240:ASP:N	2.67	0.51
1:A:230:SER:CB	1:A:279:ASN:HD21	2.24	0.51
1:A:280:GLN:O	1:A:284:GLU:HG3	2.10	0.51
1:A:467:ASP:HA	1:A:479:THR:O	2.11	0.51
1:A:126:PRO:HG3	1:A:599:TYR:CE2	2.46	0.50
1:A:253:ASN:C	1:A:253:ASN:HD22	2.19	0.50
1:A:507:MET:O	1:A:508:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:O	1:A:244:GLU:HB2	2.10	0.50
1:A:425:THR:HG23	1:A:427:GLN:H	1.76	0.50
1:A:86:ARG:HB3	1:A:86:ARG:NH1	2.26	0.50
1:A:253:ASN:ND2	1:A:255:LYS:H	2.10	0.50
1:A:503:GLN:O	1:A:507:MET:HG3	2.11	0.50
1:A:170:MET:HG3	1:A:331:LEU:O	2.12	0.50
1:A:358:ASN:C	1:A:360:PRO:HD3	2.37	0.49
1:A:178:ALA:HB1	1:A:419:LYS:HE2	1.95	0.49
1:A:79:LEU:HD23	1:A:97:LEU:HD11	1.95	0.49
1:A:230:SER:HB3	1:A:279:ASN:HD21	1.78	0.49
1:A:612:VAL:CG1	1:A:613:GLY:H	2.15	0.49
1:A:425:THR:HG23	1:A:427:GLN:NE2	2.24	0.48
1:A:472:ILE:O	1:A:473:MET:HB2	2.13	0.48
1:A:437:LEU:HD23	1:A:441:TRP:CD1	2.48	0.48
1:A:329:THR:CG2	1:A:333:LYS:HB3	2.40	0.48
1:A:180:LYS:O	1:A:184:THR:HB	2.14	0.48
1:A:111:TYR:CE2	1:A:473:MET:HG2	2.48	0.48
1:A:133:GLN:NE2	1:A:643:ASN:HB2	2.28	0.48
1:A:362:ASN:HD22	1:A:364:LEU:H	1.60	0.48
1:A:361:ASN:HB3	1:A:366:ILE:HD12	1.95	0.48
1:A:250:PRO:HA	1:A:353:TRP:CE3	2.49	0.48
1:A:763:ASP:CG	1:A:764:ASP:H	2.21	0.48
1:A:356:MET:HE3	1:A:491:ILE:CD1	2.39	0.48
1:A:362:ASN:H	1:A:365:ASN:ND2	2.11	0.47
1:A:653:GLU:C	1:A:655:LYS:H	2.22	0.47
1:A:128:ILE:HG22	1:A:132:LYS:HE3	1.96	0.47
1:A:261:PRO:HB2	1:A:262:TYR:CE1	2.50	0.47
1:A:358:ASN:ND2	2:A:1049:HOH:O	2.48	0.47
1:A:235:LEU:HD12	1:A:236:THR:H	1.78	0.47
1:A:743:ARG:HG2	1:A:743:ARG:HH11	1.80	0.47
1:A:79:LEU:HD21	1:A:276:ALA:HB2	1.97	0.47
1:A:271:ILE:HA	1:A:274:MET:HE2	1.96	0.47
1:A:187:ASN:HB3	1:A:527:ASN:HD21	1.79	0.46
1:A:776:LEU:O	1:A:780:LEU:HG	2.15	0.46
1:A:389:ILE:HG21	1:A:537:ILE:HD13	1.96	0.46
1:A:65:ARG:HG3	1:A:804:VAL:HG22	1.98	0.46
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.51	0.46
1:A:261:PRO:HD3	1:A:341:PRO:HB3	1.97	0.46
1:A:429:MET:HE3	1:A:466:VAL:CG2	2.45	0.46
1:A:563:SER:H	1:A:633:ASN:HD21	1.63	0.46
1:A:142:PRO:O	1:A:143:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HD11	1:A:267:LYS:HB3	1.98	0.46
1:A:491:ILE:HG13	2:A:1044:HOH:O	2.14	0.45
1:A:510:PRO:HG3	2:A:1199:HOH:O	2.16	0.45
1:A:133:GLN:HE21	1:A:643:ASN:HB2	1.80	0.45
1:A:204:GLN:NE2	1:A:720:LEU:HD21	2.31	0.45
1:A:273:GLU:CD	1:A:273:GLU:H	2.22	0.45
1:A:208:ILE:O	1:A:211:PRO:HD3	2.17	0.45
1:A:377:PRO:HG3	1:A:573:TRP:CE2	2.52	0.45
1:A:353:TRP:HB3	1:A:354:PRO:HD3	1.98	0.45
1:A:722:THR:CG2	1:A:724:ARG:H	2.04	0.45
1:A:189:ASN:ND2	2:A:1001:HOH:O	2.49	0.45
1:A:695:LYS:HE3	2:A:1371:HOH:O	2.15	0.45
1:A:425:THR:CB	1:A:428:HIS:HD2	2.24	0.44
1:A:59:TYR:CE2	1:A:477:ILE:HG23	2.51	0.44
1:A:229:PRO:HG2	1:A:279:ASN:OD1	2.18	0.44
1:A:757:LEU:O	1:A:760:SER:HB3	2.17	0.44
1:A:215:PRO:HD3	1:A:440:GLY:O	2.17	0.44
1:A:390:LEU:O	1:A:391:ALA:C	2.59	0.44
1:A:181:GLU:HB3	2:A:1056:HOH:O	2.18	0.44
1:A:447:PRO:HG3	1:A:732:SER:HA	2.00	0.43
1:A:175:ARG:O	1:A:178:ALA:HB3	2.17	0.43
1:A:209:THR:O	1:A:371:SER:HB2	2.18	0.43
1:A:401:ALA:HB2	1:A:490:PHE:CD1	2.54	0.43
1:A:217:GLU:O	1:A:217:GLU:HG3	2.19	0.43
1:A:347:MET:HB3	1:A:456:PHE:CZ	2.54	0.43
1:A:78:ILE:HD12	1:A:78:ILE:N	2.32	0.43
1:A:145:ASN:ND2	1:A:145:ASN:C	2.77	0.43
1:A:229:PRO:HG3	1:A:278:SER:HB2	1.99	0.43
1:A:743:ARG:HB2	1:A:746:ASP:OD2	2.19	0.43
1:A:317:LEU:HB2	1:A:339:SER:HB3	1.99	0.43
1:A:527:ASN:N	1:A:527:ASN:ND2	2.66	0.43
1:A:621:VAL:HA	1:A:683:LEU:HD21	2.01	0.43
1:A:50:LEU:HD13	1:A:475:LEU:HD12	2.01	0.42
1:A:461:ALA:HB3	1:A:462:PRO:HD3	2.00	0.42
1:A:704:VAL:CG1	1:A:705:ASN:N	2.81	0.42
1:A:726:ARG:NH1	1:A:728:GLU:OE2	2.50	0.42
1:A:410:ASN:OD1	1:A:538:ARG:HG3	2.19	0.42
1:A:67:LEU:HD12	1:A:67:LEU:H	1.85	0.42
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.85	0.42
1:A:362:ASN:HB2	1:A:371:SER:O	2.20	0.42
1:A:382:LEU:HD21	1:A:575:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:SER:HB2	1:A:477:ILE:O	2.20	0.42
1:A:176:LEU:HD11	1:A:318:LEU:CD2	2.50	0.41
1:A:184:THR:HG22	1:A:185:GLY:N	2.34	0.41
1:A:679:PHE:O	1:A:680:ASN:C	2.63	0.41
1:A:70:ASN:HA	1:A:99:LEU:O	2.20	0.41
1:A:74:GLU:O	1:A:77:GLN:HB2	2.20	0.41
1:A:61:VAL:HG22	1:A:477:ILE:CD1	2.51	0.41
1:A:253:ASN:C	1:A:253:ASN:ND2	2.79	0.41
1:A:342:SER:HB2	1:A:343:PRO:HD3	2.02	0.41
1:A:284:GLU:O	1:A:288:LEU:HD22	2.20	0.41
1:A:391:ALA:HB1	1:A:393:GLU:OE1	2.21	0.41
1:A:184:THR:CG2	1:A:185:GLY:N	2.84	0.41
1:A:229:PRO:HG3	1:A:278:SER:CB	2.50	0.41
1:A:727:ASN:O	1:A:766:ASP:HB3	2.20	0.41
1:A:191:ASP:OD2	1:A:427:GLN:HG3	2.19	0.41
1:A:506:LEU:CD1	1:A:721:LYS:HD3	2.51	0.40
1:A:61:VAL:HA	1:A:477:ILE:HD13	2.02	0.40
1:A:177:VAL:HG22	2:A:1101:HOH:O	2.21	0.40
1:A:751:LYS:O	1:A:754:ALA:HB3	2.21	0.40
1:A:145:ASN:HD22	1:A:147:GLY:H	1.69	0.40
1:A:237:GLY:C	1:A:239:VAL:H	2.30	0.40
1:A:67:LEU:HD13	1:A:106:TYR:CE2	2.57	0.40
1:A:329:THR:CG2	1:A:329:THR:O	2.68	0.40
1:A:410:ASN:ND2	1:A:536:ASP:HA	2.37	0.40
1:A:504:TRP:HD1	1:A:510:PRO:HD2	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:CB	1:A:144:ALA:CB[10_666]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	761/774 (98%)	709 (93%)	44 (6%)	8 (1%)	11	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	VAL
1	A	221	PRO
1	A	238	ASP
1	A	244	GLU
1	A	420	GLY
1	A	789	VAL
1	A	143	GLU
1	A	487	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	657/666 (99%)	627 (95%)	30 (5%)	24	48

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	65	ARG
1	A	67	LEU
1	A	152	VAL
1	A	177	VAL
1	A	209	THR
1	A	210	LEU
1	A	212	VAL
1	A	273	GLU
1	A	288	LEU
1	A	296	LYS

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Mol	Chain	Res	Type
1	A	324	ARG
1	A	329	THR
1	A	347	MET
1	A	362	ASN
1	A	365	ASN
1	A	425	THR
1	A	427	GLN
1	A	489	THR
1	A	495	LEU
1	A	500	VAL
1	A	511	ARG
1	A	518	LYS
1	A	527	ASN
1	A	531	GLU
1	A	568	LEU
1	A	629	VAL
1	A	718	ASN
1	A	744	LEU
1	A	745	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	70	ASN
1	A	122	ASN
1	A	140	GLN
1	A	145	ASN
1	A	158	ASN
1	A	189	ASN
1	A	204	GLN
1	A	253	ASN
1	A	280	GLN
1	A	291	GLN
1	A	299	ASN
1	A	362	ASN
1	A	365	ASN
1	A	427	GLN
1	A	428	HIS
1	A	493	ASN
1	A	527	ASN
1	A	633	ASN

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Mol	Chain	Res	Type
1	A	651	HIS
1	A	694	ASN
1	A	703	ASN
1	A	745	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	765/774 (98%)	0.50	85 (11%) 10 8	27, 42, 89, 126	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	8.0
1	A	243	PHE	6.7
1	A	612	VAL	6.1
1	A	239	VAL	5.7
1	A	220	LYS	5.5
1	A	144	ALA	5.2
1	A	217	GLU	5.2
1	A	241	GLY	4.9
1	A	92	VAL	4.4
1	A	763	ASP	4.4
1	A	765	PRO	4.3
1	A	710	THR	4.3
1	A	723	GLY	4.3
1	A	143	GLU	4.2
1	A	261	PRO	4.1
1	A	260	LEU	4.1
1	A	185	GLY	4.0
1	A	236	THR	4.0
1	A	789	VAL	4.0
1	A	613	GLY	3.9
1	A	654	ALA	3.9
1	A	706	ARG	3.8
1	A	84	TRP	3.6
1	A	88	ILE	3.6
1	A	707	PRO	3.6
1	A	722	THR	3.4
1	A	791	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	TYR	3.3
1	A	221	PRO	3.3
1	A	238	ASP	3.3
1	A	91	ALA	3.2
1	A	240	ASP	3.2
1	A	679	PHE	3.2
1	A	759	LYS	3.2
1	A	31	LEU	3.0
1	A	656	GLY	3.0
1	A	184	THR	2.9
1	A	761	LYS	2.9
1	A	657	PHE	2.9
1	A	708	VAL	2.9
1	A	513	ASP	2.9
1	A	234	VAL	2.8
1	A	245	VAL	2.8
1	A	762	PRO	2.8
1	A	655	LYS	2.8
1	A	87	GLN	2.7
1	A	219	ASP	2.6
1	A	216	GLY	2.6
1	A	790	ALA	2.6
1	A	93	LEU	2.6
1	A	235	LEU	2.6
1	A	658	PRO	2.5
1	A	711	GLY	2.5
1	A	764	ASP	2.5
1	A	104	GLN	2.5
1	A	770	PHE	2.5
1	A	709	ASN	2.5
1	A	678	GLY	2.4
1	A	680	ASN	2.4
1	A	222	TRP	2.4
1	A	244	GLU	2.3
1	A	724	ARG	2.3
1	A	218	ASP	2.3
1	A	242	ASP	2.3
1	A	252	ILE	2.2
1	A	721	LYS	2.2
1	A	85	MET	2.2
1	A	516	GLU	2.2
1	A	614	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	766	ASP	2.2
1	A	94	LYS	2.2
1	A	681	ILE	2.2
1	A	615	GLU	2.2
1	A	767	ALA	2.1
1	A	784	ASP	2.1
1	A	756	LYS	2.1
1	A	760	SER	2.1
1	A	668	GLU	2.1
1	A	782	LYS	2.1
1	A	443	ASP	2.1
1	A	83	ALA	2.0
1	A	650	ARG	2.0
1	A	298	SER	2.0
1	A	653	GLU	2.0
1	A	442	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.